100 YEARS AGO

A deputation of representatives from the Decimal Association, chambers of commerce, educational institutions, and trade unions, waited upon Mr. Ritchie on Wednesday, March 22, at the House of Commons to urge upon the Government the compulsory adoption of the metric system of weights and measures on January 1, 1901. Several of the delegates described the advantages which the metric system possesses, reference being made to the great waste of time involved in teaching our complicated system of arithmetic, and the loss of trade resulting from the use of a system not understood by other nations. In reply, Mr. Ritchie expressed himself in agreement with the arguments in favour of the metric system, but stated that his own view, and that of his colleagues, was that chaos and confusion would be created by the compulsory adoption of the metric system in this country, and it would be practically impossible to carry out a compulsory law on the subject. They had not only passed a law two years ago to make the metric system legal, but they had also added to their Board of Trade standards the standards for the metric system, and only seventeen of the whole of the local authorities in the country had come to verify their standards.

From *Nature* 30 March 1899.

50 YEARS AGO

'Earthquake Willis', one of the most colourful and widely known figures in American geology, has passed away. ... For him the theory of continental drift was "a fairy tale, ein Märchen"; no need to invoke it to answer the demands of palaeontology when temporary isthmian links might do the same with less affront to his concepts of earth-mechanics. For him, the propulsive force in earth-movements was volume-change at depth, brought on by the rise of 'asthenoliths', blisters of molten rock, developed by decay of radioactive substances scattered irregularly beneath the crust. The earth is growing hotter; the rising blisters expand upward, and their covering rocks, becoming foliated by recrystallization, spread sideways. Discoidal surfaces of shear form in the lithosphere; the disks rise and fall. Metamorphism is no less the cause than the result of orogeny.

From *Nature* 2 April 1949.

and theoretical work on host–parasite dynamics is relatively new; this explains why the work by Hudson *et al.* is so recent, but not the vole cycle study. Part of the explanation is surely that such large-scale experimental studies, working with complicated systems in the field, are very difficult. But I suspect that part of the reason is that these kinds of studies are necessarily a bit messy and imprecise, lacking the crisply controlled accuracy of a study on a 10-m^2 plot which too often seems more glibly 'scientific' to a funding agency. There have indeed been many such studies of population cycles in tiny enclosures, and they have not taught us a lot. I cheerfully see studies such as those described here as part of a growing recognition that important ecological questions simply have to be addressed on the right scale — which often means an uncomfortably large scale — even if that means accepting a certain degree of imprecision. □

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Semiconductor physics

Phonons rewrite structural recipes

Mark S. T. Bukowinski

The well-developed physics of semiconductors has given scientists fast computers and experimental equipment capable of measurements with high resolution. So it is fitting that, by applying these very tools, physicists have discovered that the domain of semiconductor crystal structures, and the processes responsible for them, is far richer than indicated by the models upon which the advances were built. First, there were new high-pressure angle-dispersive X-ray measurements, which showed that some of the previously predicted and apparently observed structures did not exist[1]. Now, writing in *Physical Review Letters*, Ozoliņš and Zunger[2] show that calculations from first principles may give the wrong structures when such calculations are only based upon the 'usual suspects'. The authors used fast computers to incorporate the effects of phonons — which are quanta of crystal lattice vibrations — into the theory, and discovered that the old standby structures do not stand up well to atomic vibrations.

The prototypical semiconductor is part of the family of $A^N B^{8-N}$ compounds, where A and B are elements in the N^{th} and $(8-N)^{\text{th}}$ main groups of the periodic table. For example, gallium arsenide (GaAs) and indium phosphide are $A^{\text{III}}B^{\text{V}}$ compounds. Observations and simple theoretical models based on concepts of ionic size, as well as the relative electronegativity (power of the atoms to attract electrons) and hence the degree of covalency or ionicity of the chemical bonds, yield three dominant structure types for these compounds[3]. Those in which the energy benefits of forming four, fully saturated covalent bonds outweigh the competing need for efficient atomic packing, adopt tetrahedrally coordinated structures. These 'covalent' structures include the diamond lattice of elemental semiconductors such as silicon and germanium, and the zinc blende or wurtzite structures of many $A^{\text{III}}B^{\text{V}}$ and $A^{\text{II}}B^{\text{VI}}$ compounds. Those 'ionic' compounds with ionicities that exceed about 80% tend to adopt the octahedral coordination of the sodium chloride (NaCl) structure. The semimetallic tin adopts a third 'metallic' structure, β-tin. This is also octahedrally coordinated, although the four equatorial bonds are somewhat distorted towards tetrahedral corners, suggesting a significant covalent influence. Pseudopotential calculations from first principles, which involve solutions of Schrödinger's wave

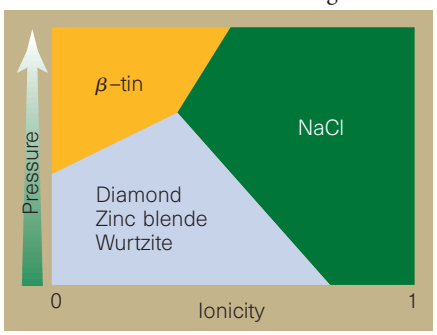

Figure 1 **Schematic phase diagram showing how the structures of most of the $A^N B^{8-N}$ octet semiconductors were found to depend on bond ionicity and pressure. (The pressure scale is of the order of 10 GPa.) Detailed structural information, made possible by the combination of synchrotron X-rays with high-pressure diamond-anvil devices, revealed that only silicon and germanium adopt the β-tin structure at high pressure, and that many of the purported NaCl phases do not exist. Observed structures have lower symmetry, often corresponding to distortions of the NaCl or β-tin structures.**

equation without any empirically adjustable parameters (only carefully developed approximations of a 'mean field' type are allowed to convert the intractable many-electron problem to a single-electron problem), have largely supported the three-structure model[4].

This simple picture appeared to remain intact when some of the compounds were subjected to high pressures. Although pressure lowers ionicity, the NaCl structure offers the advantage of higher coordination of atoms and hence more efficient atomic packing, as does the β-tin structure. So a simple phase diagram was born (Fig. 1). Again, electronic structure calculations from first principles were consistent with observations and earlier model predictions[4]. Highly covalent compounds were found to transform directly to the β-tin structure, whereas more ionic ones encountered the NaCl structure as an intermediate phase.

Hints that our traditional understanding might be incomplete emerged in the late 1970s. The semiconductor GaAs was found to transform at a pressure of 17 gigapascals (GPa) into an orthorhombic phase[5], rather than the expected β-tin. (Atmospheric pressure is approximately equal to 10^5 Pa.) When forced to examine other possible structures, theorists found one[6] with lower optimal energy than those of the NaCl and β-tin. It is now known that this structure, which can be derived from NaCl by slight displacements of alternate NaCl lattice planes, has a symmetry described by the *Cmcm* space group.

Such distortions were not included in earlier computations, because the slower computers used then did not encourage lengthy and memory-hungry calculations that minimize energy with respect to multiple degrees of freedom. So theoreticians would minimize the energy of the three prototypical structure types (the usual suspects) within the restricted space of those crystal parameters that would not change the crystal structure, such as the lattice constant of NaCl. The results were satisfying and encouraging, as they accorded with the canonical phase diagram.

As the saying goes, you get what you pay for. Energy optimizations in a restricted parameter space can only yield structures that are consistent with those restrictions. Figure 2 illustrates the potential penalties; structures with different symmetry will be missed. As bad luck would have it, the X-ray spectrum of a slightly distorted structure differs from the undistorted one by small splittings of certain spectral lines. Until recently such splittings were not resolvable. It is ironic that, despite the fact that distortions of this type are common among known solids[7], it is limitations in semiconductor technology (among others) that, by restricting techniques in computational and experimental semiconductor physics, caused both to see the same limited structural menagerie.

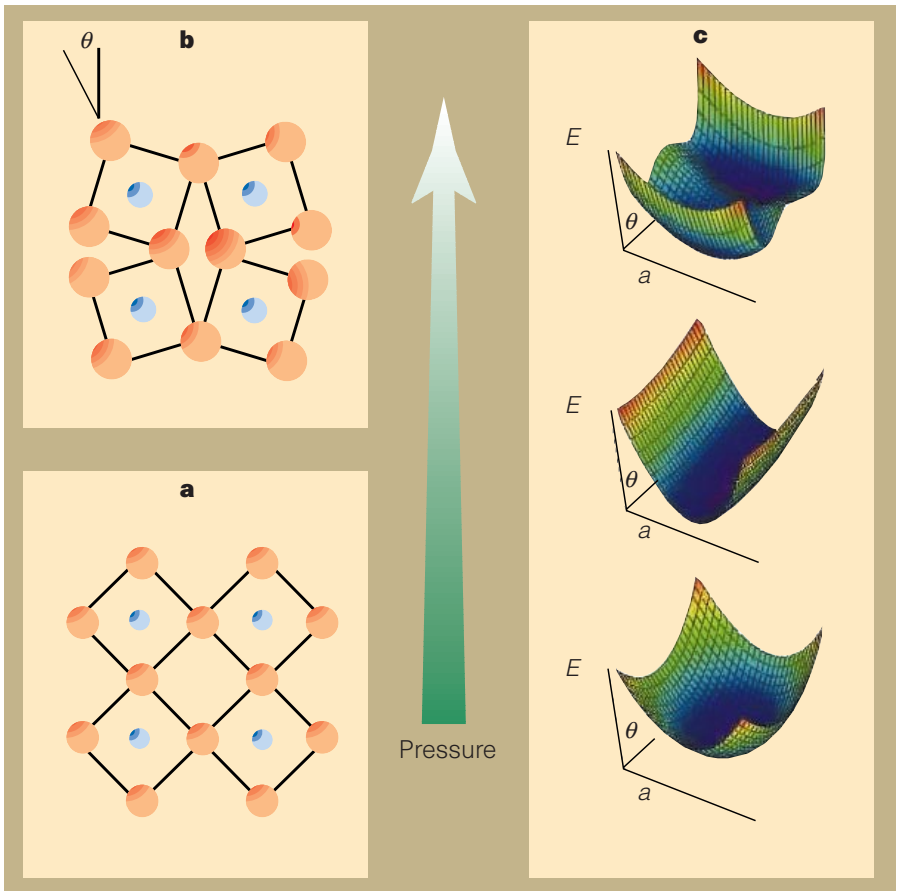

Figure 2 **Hypothetical two-dimensional crystal structure and associated energy surfaces.** a, **Equilibrium low-pressure structure has square symmetry.** b, **At high pressure the structure distorts by way of linked rotations, through angle θ, of the square coordination 'polyhedra'.** c, **The energy surface as a function of the lattice constant *a*, which is the side length of the unit cell consisting of four polyhedra, and θ. At zero pressure the surface has a minimum at $\theta = 0$. Optimization with respect to *a* alone yields the correct structure. At intermediate pressures the structure is still square, but the energy depends weakly on θ. At high pressures, restricted optimizations still yield a square lattice; but because the $\theta = 0$ extremum has now become an unstable saddle point (maximum with respect to θ), the lattice distorts in response to any perturbation in θ, such as would be created by a lattice vibration. The squared frequency of the corresponding phonons decreases with pressure because the restoring force (which is proportional to the curvature of the energy along θ) diminishes until, at some critical pressure, the force disappears altogether, and atomic displacements proceed until one of the flanking stable minima is found. The new structure may reflect additional distortions as in** b, **where the structure shrinks along the horizontal direction, giving two distinct lattice constants.**

And yet the results reported by Ozoliņš and Zunger[2] capitalize on recent computational advances. By computing phonon spectra from first principles for several semiconductors, the authors suggest that the NaCl and β-tin structures have intrinsic dynamical instabilities. In NaCl there appears to be a transverse acoustic phonon whose frequency decreases with pressure. So, although the NaCl structure of gallium phosphide is found to be energetically stable relative to the zinc blende structure at pressures exceeding 1.68 GPa, by then the NaCl structure is dynamically unstable. Interestingly, the β-tin instabilities are caused by soft phonons whose frequencies increase with pressure, suggesting that this structure might become stable at higher pressures. The net outcome is a structurally more diverse family of semiconductors.

Time will tell whether the theoretical details are accurate. There is good correspondence between the latest experimental structures and the results reported by Ozoliņš and Zunger. Whatever the outcome, the new theoretical and computational capabilities greatly improve the quantum-mechanical structural microscope. This will benefit all those who search for new materials or who try to divine the mineral composition of planetary interiors, as well as enhancing our understanding of everyday materials such as semiconductors. □

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Developmental biology

A unity of opposites

Ethan Bier

During development, cells secrete factors — referred to as morphogens — that influence the fates of their neighbours. These morphogens are distributed across groups of cells in a graded fashion, eliciting distinct responses depending on their concentration. Because morphogens are critical for initiating many patterning processes, there has been much interest in how they act at various distances to activate or suppress gene expression. We know that, in some cases, morphogens act over short distances (one to five cells); in others they influence cell fates over a much longer range (10–30 cells). Now, Ashe and Levine[1] (page 427 of this issue) provide the first evidence that a morphogen known as Short gastrulation (Sog) exerts different effects at short versus long range.

Sog is involved in patterning the dorsal–ventral axis of the early fruitfly embryo[2–4] at what is known as the blastoderm stage, when all cells seem to be morphologically equivalent. It is thought to do so by opposing the action of another morphogen called Decapentaplegic (Dpp)[3–5], a secreted protein[6] that belongs to the family of bone-morphogenetic proteins (BMPs). Sog is expressed in the lateral cells that comprise the neuroectoderm (which contributes to formation of the nervous system), whereas Dpp is expressed in adjacent dorsal cells. These cells give rise to the dorsal epidermis and to an extra-embryonic tissue called the amnioserosa, which forms at the dorsal extremity of the embryo (Fig. 1a). There is much evidence to suggest that peak levels of Dpp signalling specify the presumptive amnioserosa, whereas lower levels define the dorsal ectoderm[7]. Within the lateral neuroectoderm, Sog blocks Dpp signalling, allowing the cells there to follow their default preference of neural development[5,8] (Fig. 1a). This action of Sog in early-blastoderm-stage embryos limits the spread of Dpp signalling into the neuroectoderm[5], by a mechanism that has been highly conserved during evolution[8,9].

How does Sog suppress Dpp signalling asymmetrically, in the dorsal region of the embryo (Fig. 1b)? One model is that, in mid-blastoderm-stage embryos, Sog diffuses dorsally from the neuroectoderm and is degraded by Tolloid (Tld) — a metalloprotease that is expressed only in dorsal cells[10]. The theory goes that, by having a separated source and sink for Sog, a stable concentration gradient is created. Accordingly, the concentration of Sog is highest in cells immediately adjacent to the neuroectoderm (that is, the dorsal ectoderm cells) and lower in cells further from the source of Sog (the amnioserosa cells). This hypothetical Sog concentration gradient is imagined, in turn, to generate a reciprocal gradient of Dpp activity, which is maximal dorsally (in the amnioserosa) and lower ventrally (in the dorsal ectoderm). Consistent with the idea that Sog diffuses dorsally and antagonizes Dpp signalling, if expression of the *sog* gene is reduced, weak loss-of-function mutants in the Dpp pathway can be rescued[3,4]. Reduced levels of *sog* also result in vertical displacement of the border between the dorsal ectoderm and the amnioserosa[5], consistent with Sog being a long-range morphogen.

But this model does not explain why *sog*$^-$ mutants largely lack amnioserosa. Early *sog*$^-$ embryos do, in fact, have an expanded primordium for the amnioserosa, but these amnioserosa cells die prematurely[2]. Perhaps cells in the domains that correspond to the future amnioserosa and dorsal ectoderm cells need to communicate, to refine and maintain the distinctions between cells created by different levels of Dpp signalling. Alternatively, Sog might promote the formation of amnioserosa cells at a distance, as well as antagonizing Dpp signalling locally (Fig. 1c). The results of Ashe and Levine[1] argue in favour of this second possibility.

Ashe and Levine uncovered a potential long-range function for Sog by expressing the *sog* gene in a stripe along the anterior–posterior axis. This clever strategy uncouples the action of Sog from other, possibly redundant, dorsal–ventral patterning elements. When the authors examined expression of a marker for peak Dpp expression, they found that Sog had two distinct effects — it suppressed expression of the Dpp marker near the stripe of Sog expression, but broadened expression at a distance from the Sog source. So, Sog seems to exert opposing effects at short versus long range.

Ashe and Levine next used the same strategy to express Sog in mutant embryos with moderate Dpp signalling in all cells. They found that the Tld protease is critical for long-range activation by Sog, yet is not required for the short-range inhibitory effect. Consistent with the need for Tld in long-range activation, a membrane-tethered form of Sog was effective only at short-range inhibition of Dpp.

The new results raise several questions. First, is the long-range positive action of Sog direct, or is it propagated by a relay mechanism? Because the authors could uncouple long-range activation from short-range inhibition, the long-range activity is probably direct. Second, what is the nature of this activity? Perhaps Sog, or a fragment generated by Tld cleavage, forms a complex with Dpp, stimulating its activity. Or maybe a form of Sog acts directly on Dpp receptors to promote signalling. Alternatively, Dpp signalling would be stimulated if Sog inhibited a BMP-related molecule that normally

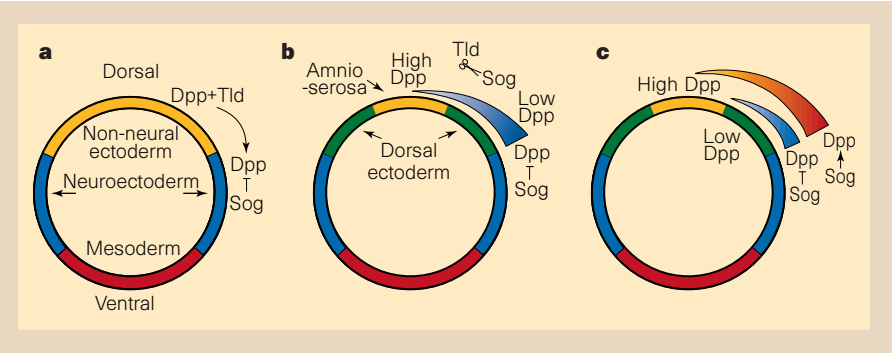

Figure 1 **Signalling by Sog.** a, **Cross-sectional view of an early-blastoderm-stage embryo. Sog is expressed in lateral cells comprising the neuroectoderm; Dpp and Tld are expressed in dorsal cells comprising the non-neural ectoderm. Sog prevents Dpp signalling from spreading into the neuroectoderm by interfering with a positive-feedback loop created by Dpp diffusing and activating its own expression[8].** b, **A mid-blastoderm-stage embryo, in which Sog signalling subdivides the dorsal region into a zone of high Dpp signalling (amnioserosa) and a zone of low Dpp signalling (dorsal ectoderm). The hypothetical Sog concentration gradient is created owing to the source of Sog in the neuroectoderm (high concentration) and its degradation by Tld in dorsal cells (low concentration). In this model, Sog only inhibits Dpp signalling.** c, **A mid-blastoderm-stage embryo in which Sog inhibits Dpp signalling locally and promotes Dpp signalling at long range, based on the results of Ashe and Levine[1].**